

Lead-free double perovskites are promising alternatives to lead-based perovskites in solar cells due to their nontoxicity, stability, and improved photovoltaic characteristics. In this work, we synthesized $\text{Na}_2\text{M}\text{BiBr}_6$ ($\text{M}=\text{Ag}, \text{Cu}$) nanoparticles following the antisolvent recrystallization method. XRD analysis revealed that the compounds lie in the $\text{Fm}\bar{3}\text{m}$ space group. The calculated lattice parameters of $\text{Na}_2\text{AgBiBr}_6$ and $\text{Na}_2\text{CuBiBr}_6$ were found to be 10.78 and 10.66 Å, respectively. SEM was performed to analyze sample surface morphology, resulting in an average particle size of 0.2 and 0.15 μm . The EDX analysis demonstrated the qualitative and quantitative elemental composition of both materials. The presence of functional groups and the chemical bonding were studied using FTIR spectroscopy. The compounds were also evaluated for various properties using Wien2K code. Both perovskites exhibited stability in cubic structure with tolerance factor (τ) values of 0.78 and 0.76, respectively. Negative formation energy values of -2.28 eV/atom and -2.66 eV/atom and Gibbs free energies of -1.03×10^7 kJ/mol and -1.12×10^8 kJ/mol confirmed their thermodynamic stability. The evaluated elastic properties helped calculate the mechanical stability. In contrast to brittle $\text{Na}_2\text{CuBiBr}_6$, $\text{Na}_2\text{AgBiBr}_6$ was ductile, having Poisson's ratio value of 0.306 (> 0.26) and high anisotropy. The electronic band gap and density of states calculations confirmed the presence of an indirect band gap (E_g) having values of 2.2 and 1.57 eV, respectively. The high absorption coefficient and low reflectivity of both materials in the visible region hold notable importance in solar cell applications. The BoltzTraP code was utilized to compute the thermoelectric properties. Results reveal that $\text{Na}_2\text{AgBiBr}_6$ and $\text{Na}_2\text{CuBiBr}_6$ exhibit higher figure-of-merit (ZT) up to 0.86 and 0.77, respectively. Hence, both perovskites are potential materials for future renewable energy applications including solar cells and thermoelectric devices.